

5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione
61346-87-0 | DTXSID60818264

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.32e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.59e-01

Confidence level: 4.41e-01

Nearest Neighbors from the Training Set

Image not found

1-Benzyl-5-methyl-1H-pyrimidine-2,4-dione

Measured: 5.55e-03

Predicted: 1.97e-03

Image not found

Lenacil

Measured: 2.56e-05

Predicted: 1.78e-04

Image not found

Metharbital

Measured: 9.99e-03

Predicted: 1.04e-02